Compounds (AIST, Japan), the *Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra* (Pouchert and Behnke, Eds., Aldrich Chemical Company, Volumes 1-3, 1993), *Spectral Data of Steroids* (Frenkel and Marsh, eds., Thermodynamics Research Center: College Station, 1994), and the NIST MS database software version 1.6. Experimental ^{13}C NMR and EI MS data for five compounds were obtained using standard methods.

Please replace the paragraph appearing at page 47, lines 9-18 with the following paragraph.

The biodegradation data for many monocyclic chlorobenzene derivatives in sediment may be found in the Database for Environmental Fate of Chemicals (AIST, Japan). Additional data on the biodegradability is published in *Biodegradation and Bioaccumulation Data of Existing Chemicals Based on the CSCL,* Japan Chemical Industry Ecology-Toxicology & Information Center (JETOC), Tokyo, Japan, 1992. The half-life period is used as the endpoint for the establishment of the SDAR and compounds are classified into two endpoint classes as readily biodegradable (R) (half-life < 30 days) and not readily biodegradable (NR) (half-life >30 days). The endpoint data for 34 chlorobenzene derivatives are given in Table 3 below.

Please replace the paragraph appearing at page 49, lines 1-8 with the following paragraph.

Spectral data for these chlorobenzene compounds is obtained from the Integrated Spectral Data Base System for Organic Compounds (AIST, Japan), the *Aldrich Library of ^{13}C and ^{1}H FT NMR Spectra* (Poucher and Behnke, Eds., Aldrich Chemical Company, Volumes 1-3, 1993) and the NIST MS database software version 1.6. Experimental ^{13}C NMR, EI MS, and IR data is collected when spectral data is not available in a database. Experimental spectral data is collected using standard spectroscopic protocols.

Please replace the paragraph appearing at page 51, lines 20-28 with the following paragraph.

Phototosensitized oxidations involving singlet oxygen, a strong oxidant, are implicated in photodynamic inactivation of viruses and cells, in phototherapy for cancer, in photocarcinogenesis and in photodegradation of dyes and polymers. Quenching of excited

singlet and triplet states of many substances by ground state molecular oxygen produces singlet oxygen; the lowest electronically excited singlet state of molecular oxygen. A compilation of the quantum yields for the formation of singlet oxygen in fluid solutions for over 700 substances is available from the Notre Dame Radiation Laboratory – Radiation Chemistry Data Center.

Please replace the paragraph appearing at page 56, lines 1-8 with the following paragraph.

For each of the structures generated using the combinatorial chemistry software, ^{13}C NMR spectra are predicted. The ^{13}C NMR spectra may be predicted by any known method. Examples of methods for predicting ^{13}C NMR spectra include the neural network methods described by Kvasnicka (Kvasnicka, V., *J. Math. Chem.*, **6**: 63-76, 1991) and the quantum mechanical calculations of Dios et al. (Dios et al., *Science* **260**:1491-1496, 1993). Software for predicting ^{13}C NMR spectra is also available from Advanced Chemistry Development, Toronto, Ontario, Canada (ACD/CNMR Spectrum Generator).

Please replace the paragraph appearing at page 63, lines 3-10 with the following paragraph.

In another embodiment of the invention, ^{13}C NMR spectral data are predicted by calculation (see, for example, Dios et al., *Science* **260**:1491-1496, 1993 and Kvasnicka, V., *J. Math. Chem.*, **6**: 63-76, 1991) and used in an SDAR model that has been trained on true ^{13}C NMR spectral data. Software for predicting ^{13}C NMR spectra is also available from Advanced Chemistry Development, Toronto, Ontario, Canada (ACD/CNMR Spectrum Generator). Predicted ^{13}C NMR spectral data may be used, for example, to aid in rational drug design by allowing proposed structures to be tested for potential activities before synthesis is attempted.

Please replace the paragraph appearing at page 66, lines 15-23 with the following paragraph.

Statistical methods include Principal Component Analysis (PCA) and variations of PCA such as linear regression analysis, cluster analysis, canonical variates, and discriminant analysis, soft independent models of class analogy (SIMCA), expert systems, and auto spin (see, for example, Harrington, *RESolve Software Manual*, Colorado School of Mines, 1988, incorporated